



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:40 AM UTC

PDB ID : 3AJI / pdb_00003aji
Title : Structure of Gankyrin-S6ATPase photo-cross-linked site-specifically, and incorporated by genetic code expansion
Authors : Sato, S.; Mimasu, S.; Sato, A.; Hino, N.; Sakamoto, K.; Umehara, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2010-06-07
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

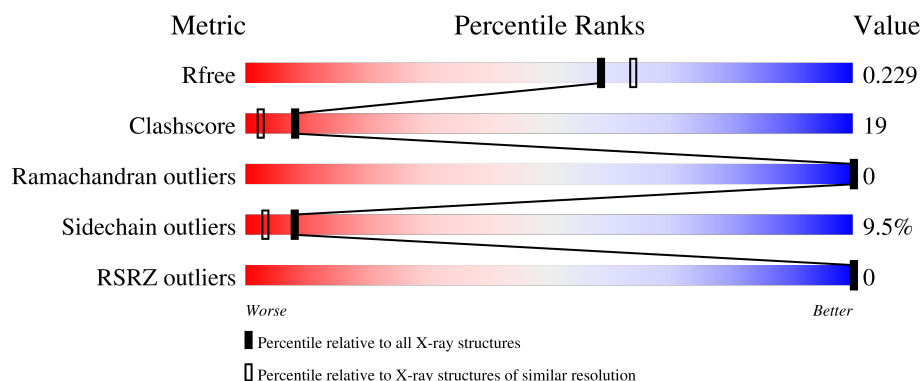
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

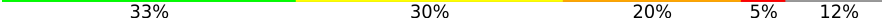
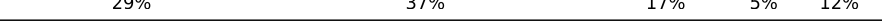
The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	231	
1	C	231	
2	B	83	
2	D	83	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4995 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 26S proteasome non-ATPase regulatory subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1745	1092	306	337	10			
1	C	229	Total	C	N	O	S	0	0	0
			1745	1092	306	337	10			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	PBF	ARG	engineered mutation	UNP Q9Z2X2
C	85	PBF	ARG	engineered mutation	UNP Q9Z2X2

- Molecule 2 is a protein called Proteasome (Prosome, macropain) 26S subunit, ATPase, 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total	C	N	O	S	0	0	0
			589	368	103	114	4			
2	D	73	Total	C	N	O	S	0	0	0
			589	368	103	114	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	336	MET	-	expression tag	UNP Q6ZWN9
D	336	MET	-	expression tag	UNP Q6ZWN9

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	144	Total	O	0	0
			144	144		
3	B	22	Total	O	0	0
			22	22		

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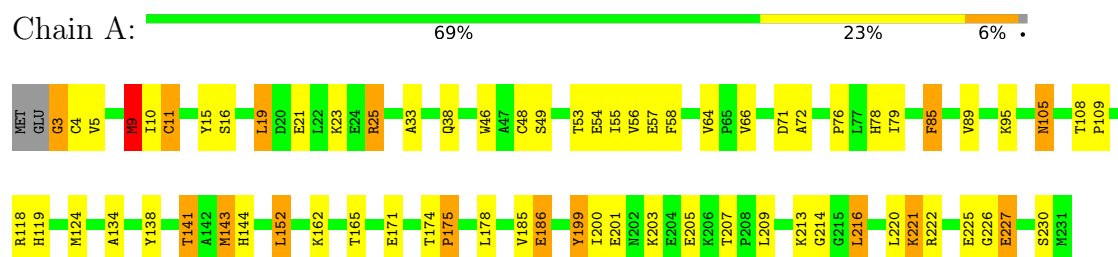
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	142	Total	O	0	0
			142	142		
3	D	19	Total	O	0	0
			19	19		

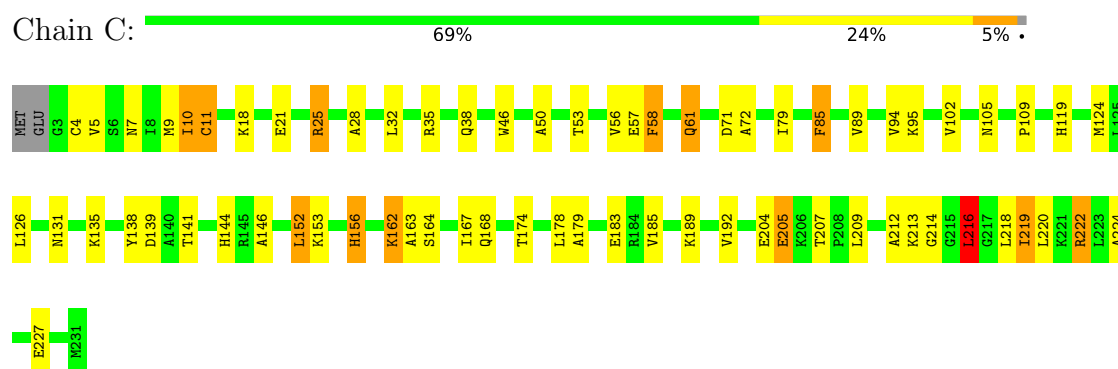
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

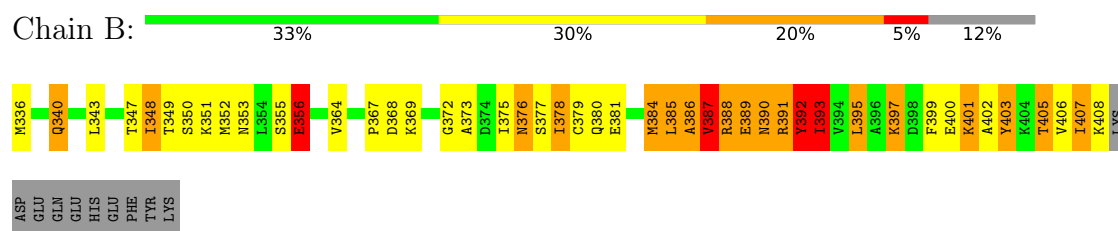
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 10



- Molecule 1: 26S proteasome non-ATPase regulatory subunit 10



- Molecule 2: Proteasome (Prosome, macropain) 26S subunit, ATPase, 4



- Molecule 2: Proteasome (Prosome, macropain) 26S subunit, ATPase, 4





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	103.16Å 103.16Å 154.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.93 – 2.05 42.93 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (42.93-2.05) 100.0 (42.93-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.05Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.171 , 0.229 0.171 , 0.229	Depositor DCC
R_{free} test set	1921 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4995	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PBF

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.85	19/1753 (1.1%)	1.56	27/2368 (1.1%)
1	C	1.88	32/1753 (1.8%)	1.55	21/2368 (0.9%)
2	B	1.85	9/594 (1.5%)	2.24	28/794 (3.5%)
2	D	1.85	12/594 (2.0%)	2.20	22/794 (2.8%)
All	All	1.86	72/4694 (1.5%)	1.75	98/6324 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
2	D	0	2
All	All	0	4

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	356	GLU	C-N	15.98	1.58	1.33
2	B	356	GLU	C-N	14.05	1.55	1.33
1	A	143	MET	SD-CE	-10.17	1.54	1.79
1	A	56	VAL	CA-CB	9.77	1.65	1.54
2	B	356	GLU	N-CA	9.03	1.57	1.46
1	C	124	MET	SD-CE	-8.33	1.58	1.79
1	A	9	MET	SD-CE	8.32	2.00	1.79
2	D	357	GLU	C-N	-8.23	1.24	1.33
2	B	356	GLU	CA-C	7.96	1.63	1.52
2	B	355	SER	C-N	-7.78	1.23	1.34
1	C	56	VAL	CA-CB	7.66	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	ALA	CA-CB	7.60	1.66	1.53
1	A	134	ALA	CA-CB	7.54	1.65	1.53
1	A	79	ILE	CA-CB	7.53	1.63	1.54
1	A	19	LEU	C-O	-7.50	1.15	1.24
2	D	395	LEU	CA-C	-7.48	1.42	1.53
1	C	9	MET	SD-CE	7.47	1.98	1.79
1	C	224	ALA	CA-CB	7.41	1.65	1.53
1	A	3	GLY	N-CA	7.25	1.57	1.45
1	A	207	THR	CA-C	7.00	1.61	1.52
1	A	124	MET	SD-CE	-6.99	1.62	1.79
1	C	207	THR	CA-C	6.86	1.61	1.52
1	A	38	GLN	C-O	-6.79	1.15	1.24
1	C	79	ILE	CA-CB	6.67	1.62	1.54
2	D	358	VAL	CA-CB	6.59	1.61	1.54
1	C	10	ILE	CA-C	6.55	1.61	1.52
2	B	395	LEU	CA-C	-6.52	1.44	1.52
1	C	179	ALA	CA-CB	6.50	1.63	1.53
1	C	50	ALA	CA-CB	6.47	1.65	1.53
1	C	164	SER	C-O	-6.28	1.16	1.23
1	C	10	ILE	CA-CB	6.25	1.63	1.54
2	D	355	SER	C-N	6.22	1.42	1.33
2	D	356	GLU	CA-CB	6.06	1.63	1.53
2	B	399	PHE	CA-C	-6.06	1.45	1.52
1	C	192	VAL	CA-CB	6.04	1.62	1.54
1	C	94	VAL	CA-C	6.01	1.60	1.52
1	C	89	VAL	CA-CB	6.01	1.61	1.54
1	C	156	HIS	N-CA	5.98	1.53	1.46
1	C	10	ILE	CB-CG1	-5.97	1.41	1.53
1	C	71	ASP	C-O	-5.96	1.16	1.24
2	D	356	GLU	CD-OE2	5.92	1.36	1.25
1	A	71	ASP	C-O	-5.91	1.15	1.24
2	D	396	ALA	CA-C	-5.88	1.44	1.52
2	B	407	ILE	CA-C	-5.77	1.47	1.53
1	C	168	GLN	C-O	-5.70	1.17	1.24
1	C	167	ILE	C-O	-5.60	1.18	1.24
1	A	10	ILE	CA-C	5.53	1.59	1.52
1	C	168	GLN	CA-CB	5.52	1.61	1.53
1	C	7	ASN	C-O	-5.51	1.16	1.24
1	C	58	PHE	CA-C	5.50	1.59	1.52
2	B	387	VAL	CA-CB	-5.46	1.47	1.54
1	C	38	GLN	C-O	-5.45	1.17	1.24
2	D	356	GLU	CG-CD	-5.44	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	396	ALA	CA-CB	-5.43	1.44	1.53
1	A	11	CYS	C-O	-5.42	1.17	1.24
1	C	131	ASN	CA-C	5.41	1.59	1.52
1	A	64	VAL	CA-C	5.37	1.58	1.52
1	C	102	VAL	CA-C	-5.33	1.46	1.52
1	A	185	VAL	CA-CB	5.27	1.60	1.54
1	C	126	LEU	C-O	-5.23	1.17	1.24
1	C	4	CYS	C-O	-5.20	1.17	1.23
1	C	25	ARG	CG-CD	-5.17	1.36	1.52
1	C	11	CYS	N-CA	5.16	1.52	1.46
1	A	109	PRO	CA-C	5.15	1.60	1.52
1	A	141	THR	C-O	5.13	1.31	1.23
2	B	356	GLU	C-O	5.12	1.30	1.24
1	C	109	PRO	CA-C	5.10	1.59	1.52
1	A	49	SER	C-O	5.07	1.30	1.24
1	A	76	PRO	CA-C	5.07	1.59	1.52
2	D	391	ARG	CZ-NH2	5.06	1.40	1.33
2	D	407	ILE	CA-CB	5.06	1.59	1.53
1	C	146	ALA	CA-C	5.05	1.59	1.52

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	390	ASN	N-CA-C	-19.45	82.86	108.34
2	B	390	ASN	N-CA-C	17.92	135.18	112.24
2	D	393	ILE	N-CA-C	-16.22	87.30	108.06
2	B	387	VAL	N-CA-C	16.12	135.16	113.07
2	D	389	GLU	N-CA-C	14.69	127.01	111.14
2	B	356	GLU	N-CA-C	-14.40	93.31	111.75
2	B	386	ALA	N-CA-C	-12.87	96.67	112.38
1	A	4	CYS	N-CA-C	12.17	128.56	111.52
2	B	356	GLU	O-C-N	-12.10	108.40	122.20
2	B	389	GLU	N-CA-C	-11.23	99.60	113.97
2	D	356	GLU	O-C-N	-11.19	107.70	122.59
2	D	392	TYR	N-CA-C	11.12	122.54	108.19
2	D	356	GLU	CB-CA-C	-9.71	91.10	110.42
2	B	355	SER	CA-C-N	9.28	133.93	120.38
2	B	355	SER	C-N-CA	9.28	133.93	120.38
2	D	391	ARG	NE-CZ-NH1	-9.24	112.26	121.50
1	C	10	ILE	CB-CG1-CD1	-8.57	95.81	113.80
2	B	378	ILE	N-CA-C	-8.15	102.49	110.72
1	A	185	VAL	N-CA-C	7.86	117.97	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	355	SER	O-C-N	7.83	132.45	122.89
2	B	389	GLU	CA-C-N	7.80	133.71	122.40
2	B	389	GLU	C-N-CA	7.80	133.71	122.40
1	C	204	GLU	N-CA-C	-7.62	104.03	112.72
2	B	377	SER	N-CA-C	7.60	119.57	111.28
1	A	199	TYR	N-CA-C	7.49	122.52	113.23
1	C	185	VAL	N-CA-C	7.27	117.40	110.42
1	C	162	LYS	N-CA-C	7.25	121.42	112.58
2	D	377	SER	N-CA-C	7.09	119.61	111.11
2	D	391	ARG	NE-CZ-NH2	7.08	125.57	119.20
2	D	392	TYR	CA-C-N	6.84	132.42	121.95
2	D	392	TYR	C-N-CA	6.84	132.42	121.95
1	A	4	CYS	CB-CA-C	-6.83	102.71	111.86
1	A	9	MET	CG-SD-CE	6.79	115.84	100.90
1	C	214	GLY	N-CA-C	6.76	120.84	112.73
2	B	372	GLY	N-CA-C	-6.75	105.99	114.16
1	C	25	ARG	NE-CZ-NH1	-6.60	114.90	121.50
1	A	213	LYS	N-CA-C	-6.56	101.87	110.53
2	B	393	ILE	N-CA-C	-6.55	98.17	108.86
1	C	174	THR	N-CA-C	-6.55	102.45	110.31
2	B	390	ASN	CB-CA-C	-6.53	101.19	111.51
1	C	119	HIS	N-CA-C	6.47	117.99	111.07
1	A	174	THR	N-CA-C	-6.37	102.66	110.31
2	B	399	PHE	N-CA-C	6.27	118.20	111.36
1	C	10	ILE	CA-CB-CG2	6.21	121.05	110.50
2	D	386	ALA	N-CA-C	-6.20	103.64	112.13
1	C	138	TYR	N-CA-C	-6.20	105.03	112.59
1	A	119	HIS	N-CA-C	6.18	117.68	111.07
2	D	373	ALA	N-CA-C	-6.15	104.27	110.97
1	A	25	ARG	NE-CZ-NH1	-6.14	115.36	121.50
1	A	162	LYS	N-CA-C	6.13	120.05	112.58
2	B	385	LEU	CB-CA-C	-6.00	98.71	110.11
1	C	227	GLU	N-CA-C	5.99	117.81	111.28
2	D	403	TYR	N-CA-C	5.98	117.47	111.07
1	A	118	ARG	NE-CZ-NH1	-5.93	115.57	121.50
1	A	138	TYR	N-CA-C	-5.93	105.36	112.59
2	D	391	ARG	CA-C-N	-5.90	111.23	122.08
2	D	391	ARG	C-N-CA	-5.90	111.23	122.08
2	D	372	GLY	N-CA-C	-5.88	105.49	113.37
1	A	72	ALA	N-CA-C	-5.88	105.30	112.88
1	A	66	VAL	CB-CA-C	-5.87	103.92	111.20
2	B	390	ASN	CA-C-N	5.81	129.61	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	390	ASN	C-N-CA	5.81	129.61	121.24
2	D	391	ARG	N-CA-C	-5.77	102.23	110.59
1	A	16	SER	CA-CB-OG	-5.76	99.59	111.10
1	C	72	ALA	N-CA-C	-5.67	106.03	113.17
1	C	5	VAL	CB-CA-C	-5.66	104.51	110.62
2	B	400	GLU	N-CA-C	-5.63	105.67	112.54
1	A	152	LEU	CB-CA-C	-5.60	102.08	110.88
1	C	212	ALA	N-CA-C	5.57	118.36	110.50
1	A	105	ASN	N-CA-C	-5.54	106.10	112.92
1	A	214	GLY	N-CA-C	5.51	120.76	113.37
1	A	108	THR	N-CA-C	-5.50	103.72	110.31
1	A	76	PRO	N-CA-C	-5.49	105.57	113.75
2	D	356	GLU	N-CA-CB	5.48	119.74	110.49
1	C	179	ALA	N-CA-C	-5.46	105.33	111.28
2	B	336	MET	CA-C-N	5.43	128.82	121.05
2	B	336	MET	C-N-CA	5.43	128.82	121.05
1	C	216	LEU	N-CA-C	-5.42	105.27	111.07
1	A	9	MET	N-CA-C	5.42	117.19	111.28
2	B	373	ALA	N-CA-C	-5.40	105.30	111.14
2	B	376	ASN	N-CA-C	-5.35	105.55	111.71
1	A	33	ALA	CA-C-N	-5.34	114.26	122.60
1	A	33	ALA	C-N-CA	-5.34	114.26	122.60
2	B	403	TYR	N-CA-C	5.34	117.80	111.33
2	B	356	GLU	N-CA-CB	5.31	118.53	110.14
2	D	357	GLU	O-C-N	-5.27	114.93	122.41
2	B	364	VAL	CB-CA-C	-5.25	105.16	112.04
1	A	200	ILE	N-CA-C	5.22	115.83	109.30
1	C	28	ALA	N-CA-C	-5.14	105.86	111.82
1	C	213	LYS	N-CA-C	-5.13	103.71	110.33
1	C	205	GLU	N-CA-C	5.12	118.83	112.58
1	A	25	ARG	CA-CB-CG	-5.12	103.87	114.10
2	D	399	PHE	N-CA-C	5.11	116.93	111.36
1	C	18	LYS	CA-C-N	5.03	126.98	120.44
1	C	18	LYS	C-N-CA	5.03	126.98	120.44
1	A	227	GLU	N-CA-C	5.03	116.76	111.28
1	A	78	HIS	CB-CA-C	-5.02	103.00	110.88
2	B	387	VAL	N-CA-CB	-5.00	100.26	111.87

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	TYR	Sidechain
2	B	392	TYR	Sidechain
2	D	363	TYR	Sidechain
2	D	399	PHE	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1745	0	1731	39	0
1	C	1745	0	1729	31	0
2	B	589	0	605	69	0
2	D	589	0	605	53	0
3	A	144	0	0	3	0
3	B	22	0	0	3	0
3	C	142	0	0	5	1
3	D	19	0	0	2	0
All	All	4995	0	4670	181	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (181) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:ASN:CG	2:B:390:ASN:O	1.84	1.16
2:D:340:GLN:HE21	2:D:340:GLN:HA	1.11	1.13
2:D:391:ARG:O	2:D:392:TYR:HD2	1.36	1.09
1:A:143:MET:HE2	1:A:175:PRO:HG2	1.37	1.07
2:D:391:ARG:N	2:D:391:ARG:HE	1.58	1.01
1:C:105:ASN:HB2	3:D:157:HOH:O	1.61	0.99
1:A:143:MET:HE1	1:A:165:THR:HA	1.45	0.98
2:D:390:ASN:C	2:D:391:ARG:HE	1.71	0.97
2:B:348:ILE:C	2:B:348:ILE:HD13	1.90	0.96
1:A:205:GLU:O	1:A:205:GLU:HG3	1.63	0.96
2:D:391:ARG:O	2:D:392:TYR:CD2	2.21	0.94
2:D:363:TYR:OH	2:D:400:GLU:HG2	1.68	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ARG:HG2	1:C:222:ARG:HH11	1.36	0.91
1:A:143:MET:CE	1:A:175:PRO:HG2	2.04	0.88
1:C:57:GLU:O	1:C:61:GLN:HG3	1.73	0.87
1:A:105:ASN:HB3	3:A:314:HOH:O	1.72	0.87
2:B:406:VAL:HG12	2:B:407:ILE:HD12	1.57	0.86
2:D:340:GLN:HA	2:D:340:GLN:NE2	1.89	0.85
1:C:32:LEU:HA	1:C:35:ARG:HD2	1.58	0.84
1:C:85:PBF:HI2	2:D:356:GLU:CD	2.05	0.81
2:B:381:GLU:O	2:B:385:LEU:HD12	1.81	0.81
1:A:85:PBF:HI2	2:B:356:GLU:CD	2.04	0.81
1:C:162:LYS:HE2	3:C:314:HOH:O	1.83	0.79
1:C:57:GLU:O	1:C:61:GLN:CG	2.32	0.77
2:B:381:GLU:HG3	2:B:385:LEU:HD11	1.67	0.76
2:D:356:GLU:HA	2:D:356:GLU:OE2	1.83	0.76
2:B:353:ASN:HD22	2:B:393:ILE:HA	1.50	0.76
1:C:183:GLU:OE2	3:C:287:HOH:O	2.04	0.76
2:D:407:ILE:O	2:D:408:LYS:HB2	1.86	0.75
1:C:222:ARG:HH11	1:C:222:ARG:CG	1.99	0.74
2:D:400:GLU:O	2:D:404:LYS:HD3	1.87	0.74
1:A:205:GLU:O	1:A:205:GLU:CG	2.36	0.74
2:B:391:ARG:HH22	2:B:397:LYS:HD3	1.53	0.73
2:D:406:VAL:HG12	2:D:407:ILE:HD12	1.71	0.72
2:B:390:ASN:O	2:B:390:ASN:OD1	2.06	0.72
1:A:105:ASN:ND2	3:A:317:HOH:O	2.22	0.72
1:A:141:THR:H	1:A:144:HIS:CD2	2.08	0.72
2:B:391:ARG:NH2	2:B:397:LYS:HD3	2.05	0.72
1:C:205:GLU:O	3:C:365:HOH:O	2.08	0.71
1:C:141:THR:H	1:C:144:HIS:CD2	2.09	0.71
2:B:376:ASN:C	2:B:380:GLN:HE21	2.00	0.69
2:D:391:ARG:N	2:D:391:ARG:NE	2.39	0.69
1:A:15:TYR:OH	2:B:393:ILE:HD13	1.94	0.68
2:B:387:VAL:HG13	2:B:390:ASN:OD1	1.94	0.68
3:C:316:HOH:O	2:D:397:LYS:HE3	1.94	0.67
2:B:348:ILE:C	2:B:348:ILE:CD1	2.66	0.67
2:D:391:ARG:NE	2:D:391:ARG:CA	2.58	0.67
2:B:391:ARG:HD2	2:B:395:LEU:HD11	1.76	0.66
1:C:141:THR:OG1	1:C:144:HIS:HD2	1.79	0.65
2:D:378:ILE:HG13	2:D:406:VAL:HG11	1.77	0.65
2:B:381:GLU:O	2:B:385:LEU:CD1	2.43	0.65
2:B:389:GLU:OE2	2:B:391:ARG:NH2	2.29	0.65
2:B:387:VAL:HA	2:B:390:ASN:HA	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:390:ASN:C	2:D:391:ARG:NE	2.51	0.64
2:B:391:ARG:NH2	2:B:397:LYS:CD	2.61	0.64
1:A:141:THR:OG1	1:A:144:HIS:HD2	1.81	0.64
1:A:53:THR:O	1:A:57:GLU:HG3	1.97	0.63
2:D:378:ILE:HD11	2:D:407:ILE:HD13	1.80	0.63
2:D:391:ARG:HE	2:D:391:ARG:CA	2.12	0.63
1:A:216:LEU:HD22	1:A:220:LEU:HG	1.80	0.62
2:B:381:GLU:HG3	2:B:385:LEU:CD1	2.30	0.62
1:A:186:GLU:HG3	1:C:153:LYS:CD	2.30	0.61
2:B:390:ASN:HB3	3:B:87:HOH:O	2.01	0.61
2:B:407:ILE:HG22	2:B:407:ILE:O	2.01	0.61
2:D:340:GLN:HE21	2:D:340:GLN:CA	1.93	0.61
1:C:61:GLN:NE2	3:C:319:HOH:O	2.33	0.60
2:B:407:ILE:O	2:B:408:LYS:HB2	2.00	0.60
2:B:378:ILE:HD11	2:B:407:ILE:HD13	1.84	0.59
2:B:391:ARG:HH22	2:B:397:LYS:CD	2.15	0.59
2:B:385:LEU:C	2:B:387:VAL:N	2.56	0.59
1:C:216:LEU:HD22	1:C:220:LEU:HG	1.84	0.59
2:B:384:MET:O	2:B:387:VAL:HG23	2.02	0.59
2:B:392:TYR:H	2:B:392:TYR:HD1	1.50	0.59
1:A:186:GLU:HG3	1:C:153:LYS:HD2	1.85	0.58
1:C:85:PBF:CI2	2:D:356:GLU:CD	2.74	0.58
1:A:143:MET:HE3	1:A:175:PRO:CB	2.33	0.58
2:B:392:TYR:CD1	2:B:392:TYR:N	2.68	0.58
2:D:343:LEU:C	2:D:343:LEU:HD13	2.28	0.58
1:A:143:MET:CE	1:A:175:PRO:CG	2.82	0.57
2:B:353:ASN:ND2	2:B:393:ILE:HA	2.20	0.57
2:D:354:LEU:HD21	2:D:399:PHE:CE1	2.40	0.57
2:B:390:ASN:CB	3:B:87:HOH:O	2.52	0.57
2:B:348:ILE:HD13	2:B:348:ILE:O	2.03	0.56
2:B:353:ASN:HD21	2:B:393:ILE:HD12	1.70	0.56
2:B:356:GLU:OE2	2:B:356:GLU:HA	2.04	0.56
2:B:401:LYS:O	2:B:405:THR:CG2	2.54	0.56
1:A:143:MET:HE3	1:A:175:PRO:HB2	1.86	0.56
1:A:186:GLU:H	1:A:186:GLU:CD	2.11	0.56
2:D:356:GLU:OE2	2:D:356:GLU:CA	2.54	0.56
2:D:341:LYS:CE	3:D:90:HOH:O	2.54	0.55
1:A:186:GLU:CG	1:C:153:LYS:HD2	2.37	0.55
1:C:222:ARG:CG	1:C:222:ARG:NH1	2.65	0.55
1:A:21:GLU:OE2	1:A:25:ARG:NH1	2.38	0.55
1:A:171:GLU:C	1:A:203:LYS:HG2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:ASN:O	2:B:380:GLN:HG3	2.06	0.55
1:A:48:CYS:O	1:A:85:PBF:HD1	2.07	0.54
2:B:376:ASN:C	2:B:380:GLN:NE2	2.64	0.54
2:D:337:ASP:C	2:D:337:ASP:OD1	2.49	0.54
2:B:401:LYS:O	2:B:405:THR:HG23	2.08	0.54
2:D:385:LEU:HG	2:D:385:LEU:O	2.08	0.53
2:D:343:LEU:HD13	2:D:343:LEU:O	2.09	0.53
2:D:353:ASN:HD22	2:D:393:ILE:HA	1.73	0.53
1:A:201:GLU:OE1	1:A:205:GLU:OE2	2.27	0.52
1:A:11:CYS:HB3	1:A:46:TRP:CD1	2.45	0.52
2:B:368:ASP:OD2	2:B:403:TYR:OH	2.16	0.52
2:B:390:ASN:ND2	3:B:87:HOH:O	2.39	0.52
1:C:57:GLU:O	1:C:61:GLN:HG2	2.10	0.52
1:A:15:TYR:HE2	2:B:392:TYR:HH	1.58	0.51
2:D:355:SER:CA	2:D:393:ILE:HD11	2.40	0.51
2:B:386:ALA:O	2:B:390:ASN:HA	2.11	0.50
2:B:353:ASN:HD21	2:B:393:ILE:CG1	2.24	0.50
2:B:392:TYR:CE1	2:B:393:ILE:HG22	2.45	0.50
2:D:384:MET:C	2:D:386:ALA:H	2.18	0.50
2:D:376:ASN:O	2:D:380:GLN:HG3	2.12	0.50
2:B:340:GLN:HE21	2:B:340:GLN:HA	1.77	0.49
2:B:401:LYS:O	2:B:402:ALA:C	2.55	0.49
1:A:221:LYS:HD3	1:A:221:LYS:C	2.36	0.49
1:A:3:GLY:HA2	2:B:392:TYR:CZ	2.48	0.49
2:B:385:LEU:O	2:B:386:ALA:C	2.55	0.49
2:B:353:ASN:ND2	2:B:393:ILE:HG13	2.28	0.48
1:A:85:PBF:CI2	2:B:356:GLU:CD	2.83	0.48
1:C:58:PHE:HA	1:C:61:GLN:HE21	1.78	0.48
2:D:376:ASN:C	2:D:380:GLN:HE21	2.22	0.48
2:D:348:ILE:HD13	2:D:376:ASN:HA	1.96	0.48
2:B:353:ASN:ND2	2:B:393:ILE:CG1	2.76	0.48
1:C:53:THR:O	1:C:57:GLU:HG3	2.13	0.48
1:A:227:GLU:O	1:A:230:SER:O	2.31	0.47
2:B:375:ILE:O	2:B:376:ASN:C	2.55	0.47
2:B:378:ILE:HD13	2:B:403:TYR:CD1	2.48	0.47
2:D:348:ILE:C	2:D:350:SER:N	2.71	0.47
2:D:376:ASN:C	2:D:380:GLN:NE2	2.72	0.47
2:D:405:THR:HG22	2:D:406:VAL:N	2.29	0.47
2:B:348:ILE:HD12	2:B:379:CYS:HB3	1.96	0.47
1:A:143:MET:HE1	1:A:165:THR:CA	2.31	0.47
1:C:189:LYS:HD3	1:C:219:ILE:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:LYS:HA	2:B:401:LYS:HD3	1.59	0.46
1:C:58:PHE:HA	1:C:61:GLN:HG3	1.97	0.46
2:B:387:VAL:O	2:B:390:ASN:HB2	2.15	0.46
1:A:141:THR:H	1:A:144:HIS:HD2	1.60	0.46
1:C:85:PBF:CI1	1:C:85:PBF:CE2	2.90	0.46
2:D:371:SER:OG	2:D:373:ALA:HB3	2.15	0.46
1:A:9:MET:HG2	3:A:315:HOH:O	2.16	0.45
1:A:85:PBF:O	1:A:89:VAL:HG23	2.17	0.45
1:C:11:CYS:HB3	1:C:46:TRP:CD1	2.51	0.45
2:D:375:ILE:O	2:D:376:ASN:C	2.59	0.45
2:B:349:THR:HA	2:B:352:MET:HG3	1.99	0.45
2:D:367:PRO:O	2:D:367:PRO:HG2	2.16	0.45
1:C:85:PBF:CE2	1:C:85:PBF:HI1	2.45	0.45
2:D:384:MET:HA	2:D:387:VAL:HG12	1.99	0.45
1:A:5:VAL:O	2:B:391:ARG:HD3	2.16	0.45
2:B:353:ASN:HD21	2:B:393:ILE:CD1	2.30	0.45
2:D:348:ILE:C	2:D:350:SER:H	2.25	0.44
1:A:23:LYS:HG2	1:A:58:PHE:CE1	2.53	0.44
2:B:347:THR:O	2:B:350:SER:OG	2.22	0.44
1:C:141:THR:OG1	1:C:144:HIS:CD2	2.66	0.44
1:C:135:LYS:HE2	1:C:139:ASP:OD1	2.18	0.44
1:C:219:ILE:HD13	1:C:219:ILE:N	2.31	0.43
2:D:354:LEU:HD21	2:D:399:PHE:CZ	2.53	0.43
1:C:152:LEU:HD22	1:C:156:HIS:CD2	2.52	0.43
2:D:390:ASN:HB2	2:D:392:TYR:CE2	2.53	0.43
2:D:336:MET:HE3	2:D:370:ILE:O	2.18	0.43
2:B:402:ALA:O	2:B:405:THR:HG23	2.19	0.42
2:D:349:THR:HG21	2:D:360:LEU:HD11	2.01	0.42
2:D:374:ASP:O	2:D:377:SER:HB2	2.19	0.42
2:B:405:THR:OG1	2:B:406:VAL:N	2.53	0.42
2:D:400:GLU:O	2:D:404:LYS:CD	2.64	0.42
2:B:386:ALA:HB1	2:B:391:ARG:O	2.20	0.42
1:A:225:GLU:O	1:A:226:GLY:C	2.61	0.41
2:B:388:ARG:HA	2:B:388:ARG:HD3	1.80	0.41
2:D:403:TYR:O	2:D:407:ILE:HB	2.21	0.41
2:D:401:LYS:O	2:D:402:ALA:C	2.63	0.41
2:B:392:TYR:HD1	2:B:392:TYR:N	2.12	0.41
2:B:387:VAL:CG1	2:B:390:ASN:OD1	2.63	0.41
2:D:336:MET:HG3	2:D:337:ASP:N	2.35	0.41
2:D:343:LEU:HD22	2:D:343:LEU:HA	1.79	0.41
2:D:378:ILE:HD11	2:D:407:ILE:CD1	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PBF:CE2	1:A:85:PBF:CI1	2.98	0.41
1:A:19:LEU:HD13	1:A:55:ILE:HG12	2.04	0.40
2:B:376:ASN:CB	2:B:380:GLN:HE21	2.35	0.40
2:B:397:LYS:HB2	2:B:397:LYS:HE2	1.92	0.40
2:B:401:LYS:O	2:B:405:THR:HG22	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:312:HOH:O	3:C:369:HOH:O[8_654]	2.07	0.13

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	226/231 (98%)	222 (98%)	4 (2%)	0	100	100
1	C	226/231 (98%)	222 (98%)	4 (2%)	0	100	100
2	B	71/83 (86%)	68 (96%)	3 (4%)	0	100	100
2	D	71/83 (86%)	68 (96%)	3 (4%)	0	100	100
All	All	594/628 (95%)	580 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	181/183 (99%)	170 (94%)	11 (6%)	17	10
1	C	181/183 (99%)	169 (93%)	12 (7%)	15	9
2	B	66/76 (87%)	50 (76%)	16 (24%)	1	0
2	D	66/76 (87%)	58 (88%)	8 (12%)	5	1
All	All	494/518 (95%)	447 (90%)	47 (10%)	8	3

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	MET
1	A	54	GLU
1	A	95	LYS
1	A	152	LEU
1	A	175	PRO
1	A	178	LEU
1	A	186	GLU
1	A	209	LEU
1	A	216	LEU
1	A	221	LYS
1	A	222	ARG
2	B	340	GLN
2	B	343	LEU
2	B	348	ILE
2	B	351	LYS
2	B	356	GLU
2	B	367	PRO
2	B	369	LYS
2	B	384	MET
2	B	387	VAL
2	B	388	ARG
2	B	391	ARG
2	B	392	TYR
2	B	393	ILE
2	B	397	LYS
2	B	401	LYS
2	B	405	THR
1	C	10	ILE
1	C	21	GLU
1	C	25	ARG

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Mol	Chain	Res	Type
1	C	61	GLN
1	C	95	LYS
1	C	152	LEU
1	C	178	LEU
1	C	209	LEU
1	C	216	LEU
1	C	218	LEU
1	C	219	ILE
1	C	222	ARG
2	D	336	MET
2	D	337	ASP
2	D	340	GLN
2	D	356	GLU
2	D	367	PRO
2	D	391	ARG
2	D	393	ILE
2	D	397	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	104	GLN
1	A	105	ASN
1	A	137	HIS
1	A	144	HIS
1	A	194	GLN
2	B	340	GLN
2	B	353	ASN
2	B	380	GLN
1	C	38	GLN
1	C	61	GLN
1	C	104	GLN
1	C	137	HIS
1	C	144	HIS
1	C	194	GLN
2	D	340	GLN
2	D	353	ASN
2	D	380	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	PBF	C	85	1,2	18,19,21	2.35	2 (11%)	19,24,28	1.77	5 (26%)
1	PBF	A	85	1,2	18,19,21	2.61	2 (11%)	19,24,28	3.24	8 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PBF	C	85	1,2	-	2/9/10/16	0/2/2/2
1	PBF	A	85	1,2	-	3/9/10/16	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	PBF	CB-CG	9.72	1.74	1.51
1	C	85	PBF	CB-CG	-6.95	1.34	1.51
1	C	85	PBF	CB-CA	4.51	1.63	1.53
1	A	85	PBF	CB-CA	4.18	1.62	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	85	PBF	CB-CG-CD2	-10.02	102.26	120.90
1	A	85	PBF	CB-CG-CD1	7.03	133.98	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	85	PBF	CB-CG-CD2	-4.01	113.44	120.90
1	C	85	PBF	CT-CN1-CZ	-3.50	101.77	113.76
1	A	85	PBF	CD2-CG-CD1	3.38	123.26	118.23
1	A	85	PBF	CE1-CD1-CG	-2.71	117.44	121.00
1	A	85	PBF	CI2-CT-CI1	2.43	121.84	118.23
1	C	85	PBF	CE2-CZ-CE1	2.38	121.77	118.23
1	C	85	PBF	CD2-CG-CD1	2.34	121.71	118.23
1	A	85	PBF	CE2-CZ-CE1	2.34	121.71	118.23
1	C	85	PBF	CB-CG-CD1	2.05	124.72	120.90
1	A	85	PBF	CE2-CD2-CG	-2.05	118.30	121.00
1	A	85	PBF	CN1-CT-CI2	-2.05	115.70	120.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	85	PBF	CA-CB-CG-CD2
1	C	85	PBF	CA-CB-CG-CD1
1	A	85	PBF	CA-CB-CG-CD1
1	A	85	PBF	CA-CB-CG-CD2
1	A	85	PBF	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	85	PBF	4	0
1	A	85	PBF	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	228/231 (98%)	-1.37	0 100 100	20, 28, 48, 104	0
1	C	228/231 (98%)	-1.36	0 100 100	20, 27, 48, 104	0
2	B	73/83 (87%)	-0.99	0 100 100	28, 52, 81, 91	0
2	D	73/83 (87%)	-0.91	0 100 100	29, 52, 84, 101	0
All	All	602/628 (95%)	-1.27	0 100 100	20, 30, 69, 104	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PBF	A	85	18/20	0.99	0.05	21,39,73,76	0
1	PBF	C	85	18/20	0.99	0.05	19,45,70,78	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.